

Overview of IH-related Projects @ Los Alamos National Laboratory

Torsten Staab

tstaab@lanl.gov

LA-UR-04-2126



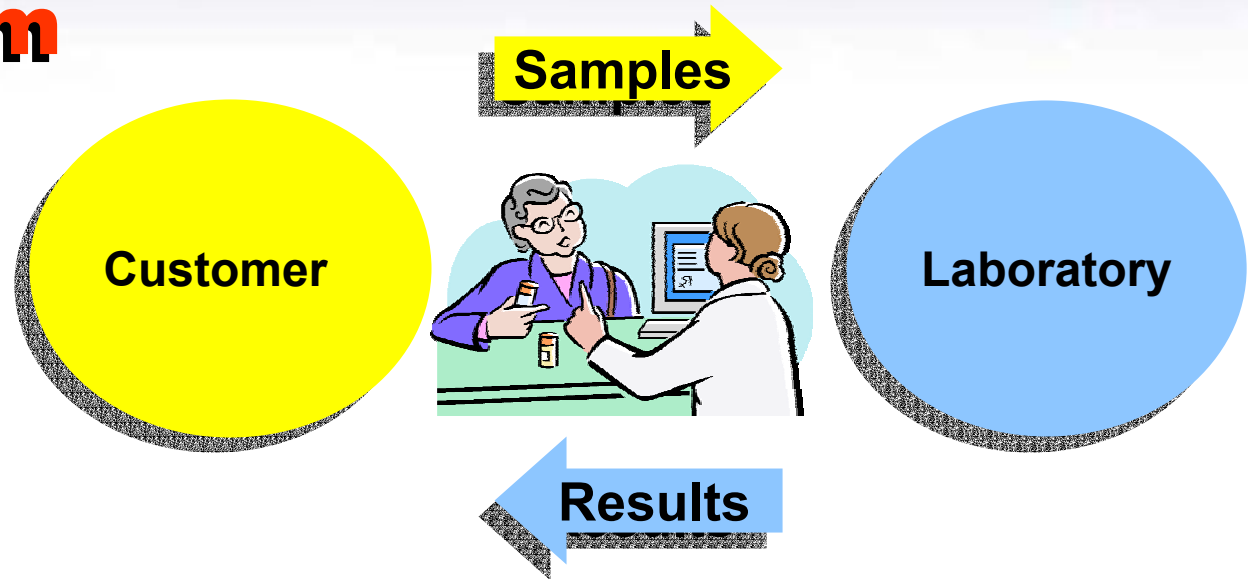
American Chemical Society National Meeting
Anaheim, CA, March 31, 2004

Agenda

- **Automating IH Records Management and Data Exchange**
- **Automated Instrument Data QC**
- **Handheld Sample Collection & Tracking Device**

Automating IH Records Management and Data Exchange

The Problem



- Use of paper forms (time consuming, requires manual validation, error prone due to re-keying, duplication of effort)
- No direct data import/export capabilities between different systems

Automating IH Records Management and Data Exchange

Our Goal

Develop data models and an information portal that enables lab- and IH folks to exchange information electronically in a platform- & system-independent manner.

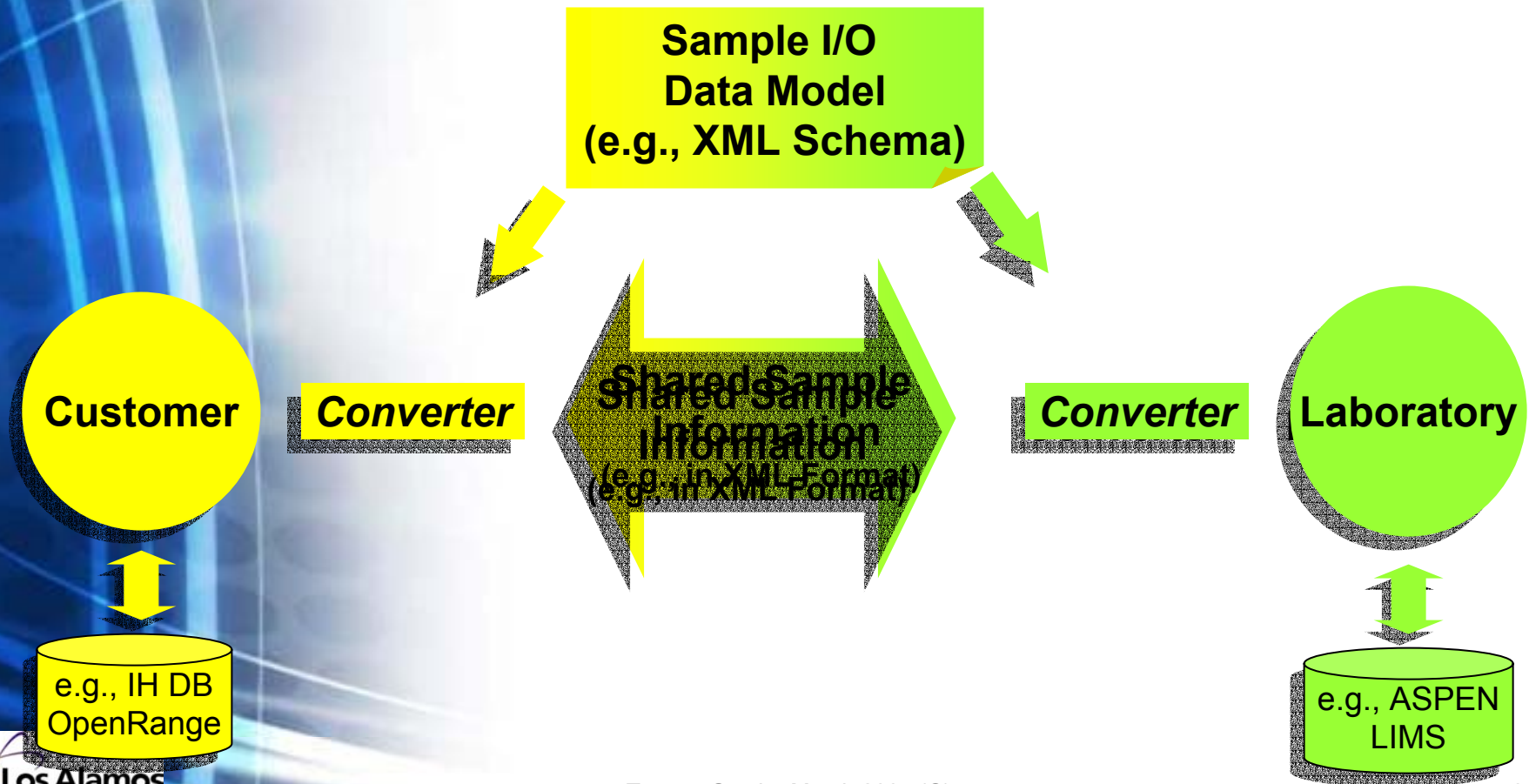
Automating IH Records Management and Data Exchange

Our Approach

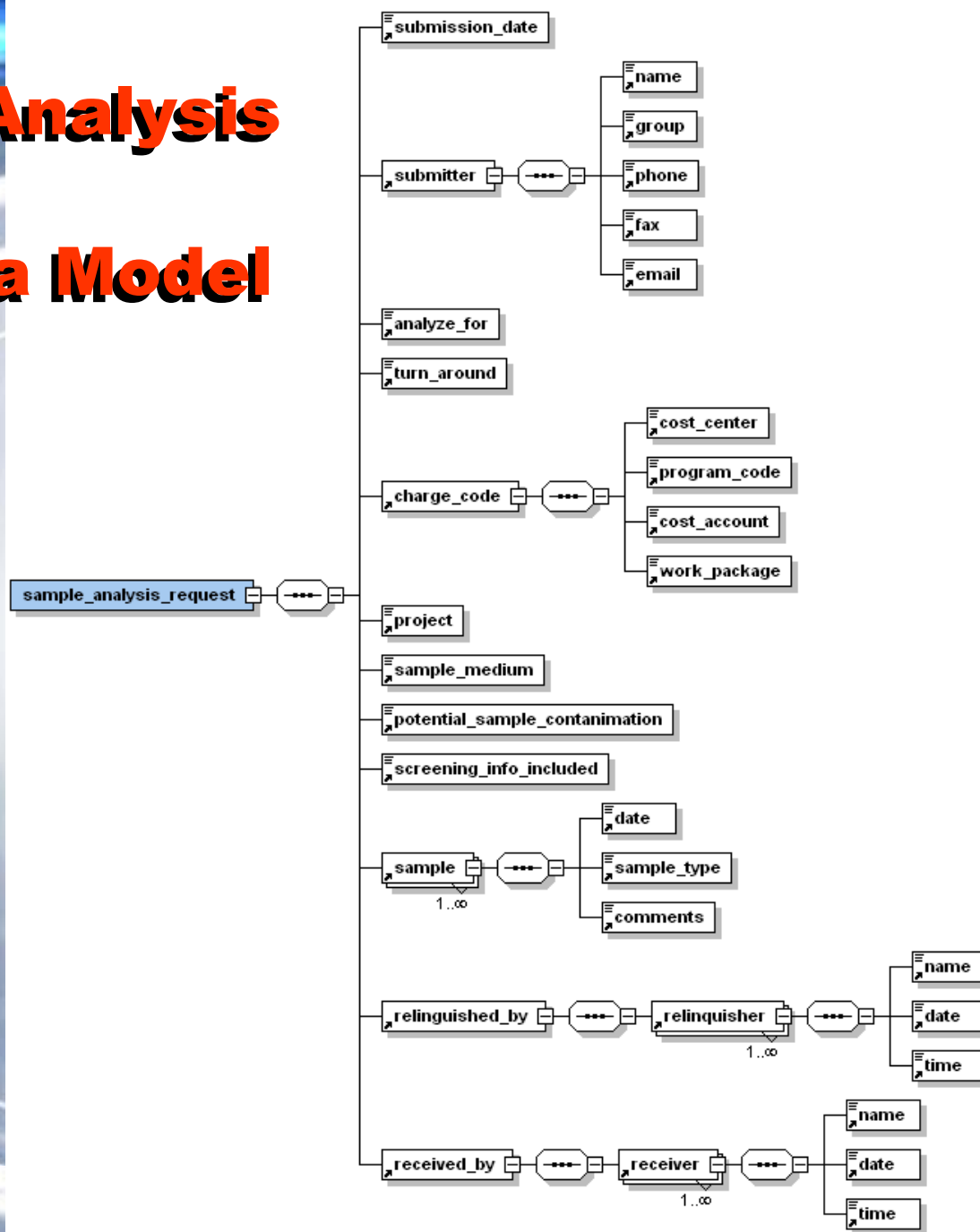
- Platform-neutral Data Modeling and Representation using **XML** (eXtensible Markup Language)
- Automate Records Management, Tracking, Approval, and Routing with **Microsoft Sharepoint**

visit <http://www.w3.org/XML/> for more info on XML

Automating IH Records Management and Data Exchange System Architecture



Sample Analysis Request XML Data Model

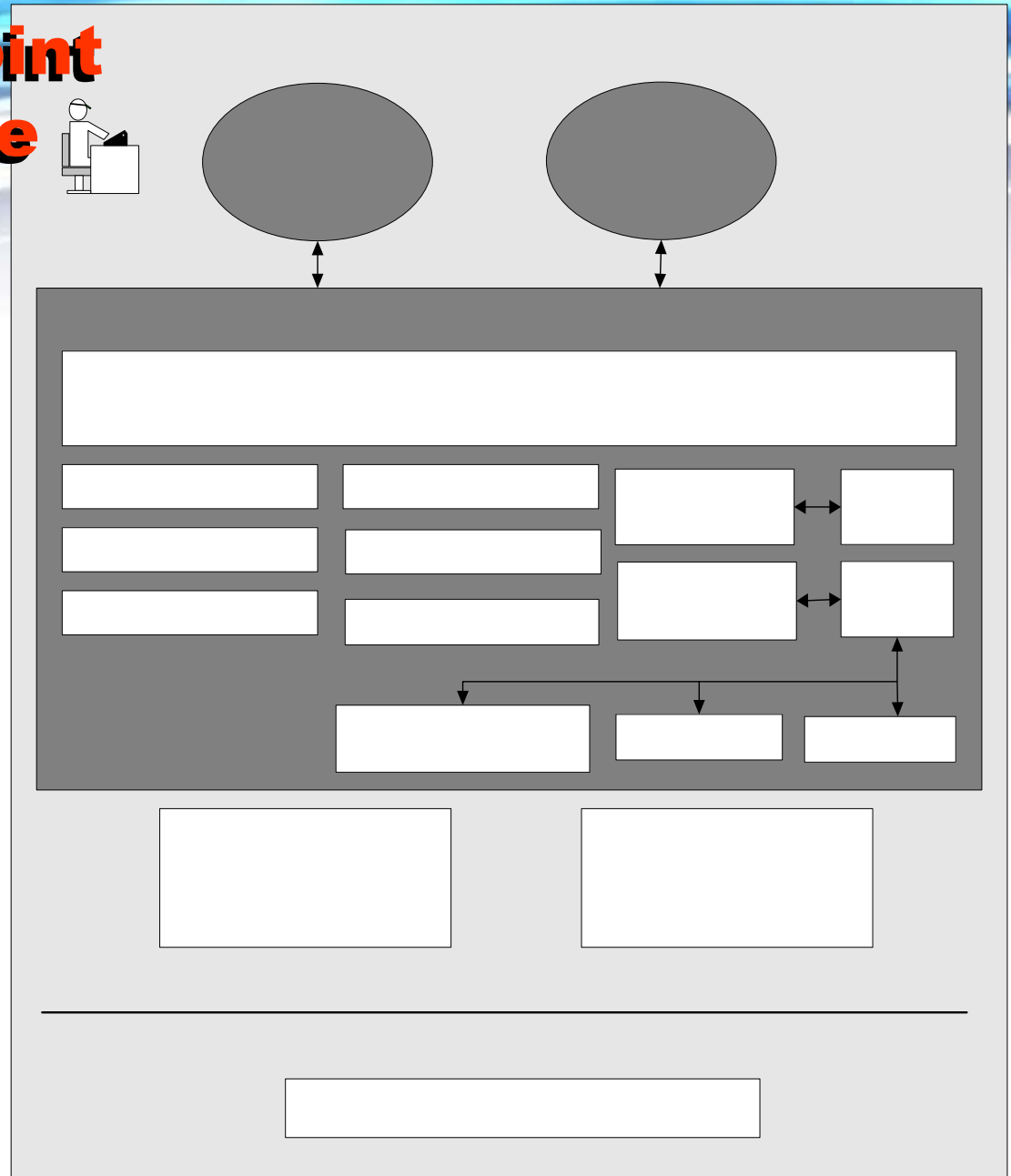


Sample Analysis Request XML Example

```
<?xml version="1.0" encoding="UTF-8" ?>
- <analysis_request id="2003-01-29_123">
  - <requester>
    <name>Alice Smith</name>
    <group>MST-6</group>
  </requester>
  - <samples>
    - <sample id="12345">
      <date_collected>01-22-04</date_collected>
      <location>TA-55 Bldg 1 R103</location>
      <media>47mm Millipore Filter</media>
      <analytesOI>Al,Be</analytesOI>
    </sample>
  </samples>
</analysis_request>
```

XML	
analysis_request	
id	2003-01-29_123
requester	
samples	
sample	
id	12345
date_collected	01-22-04
location	TA-55 Bldg 1 R103
media	47mm Millipore Filter
analytesOI	Al,Be

Microsoft Sharepoint Portal Architecture



Example: ADAPT Project Sharepoint Homepage

Home - ADAPT - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media AutoFill Options


Address http://aet-srv/sites/adapt/default.aspx Go Links

Google Search Web 446 blocked AutoFill Options

Home Documents and Lists Create Site Settings Help Up to ESA-AET

ADAPT Home

Advanced Design & Production Technologies



Electronic Data Exchange Architecture for DOE Analytical Laboratories & Industrial Hygienists

Documents

- Shared Documents
- Data Models
- Electronic Forms
- Presentations
- Correspondence

Pictures

Lists

- Contacts
- Tasks

Discussions

- General Discussion

Surveys

Tasks

Title	Assigned To
Develop Result Transfer Model NEW	Torsten A Staab

[Add new item](#)

Announcements

Uploaded sample analysis request data model and e-form 3/17/2004 3:44 PM
by Torsten A Staab
Check the **Documents** folder for the latest version of the sample analysis request data model and e-form.

[Add new announcement](#)

Events

3/24/2004 10:00 AM **IH/C-ACS Working Group Mtg**
Discuss & refine the lab output data model from last meeting.

[Add new event](#)

Los Alamos NATIONAL LABORATORY

ADAPT Project Sharepoint Documents & Lists

Documents and Lists - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media AutoFill Options

Address http://aet-srv/sites/adapt/_layouts/viewlists.aspx?BaseType=0 Go Links

Google Search Web 446 blocked AutoFill Options

Home Documents and Lists Create Site Settings Help Up to ESA-AET

ADAPT
Documents and Lists

Select a View

- All
- Document Libraries
- Picture Libraries
- Lists**
- Discussion Boards
- Surveys

See Also

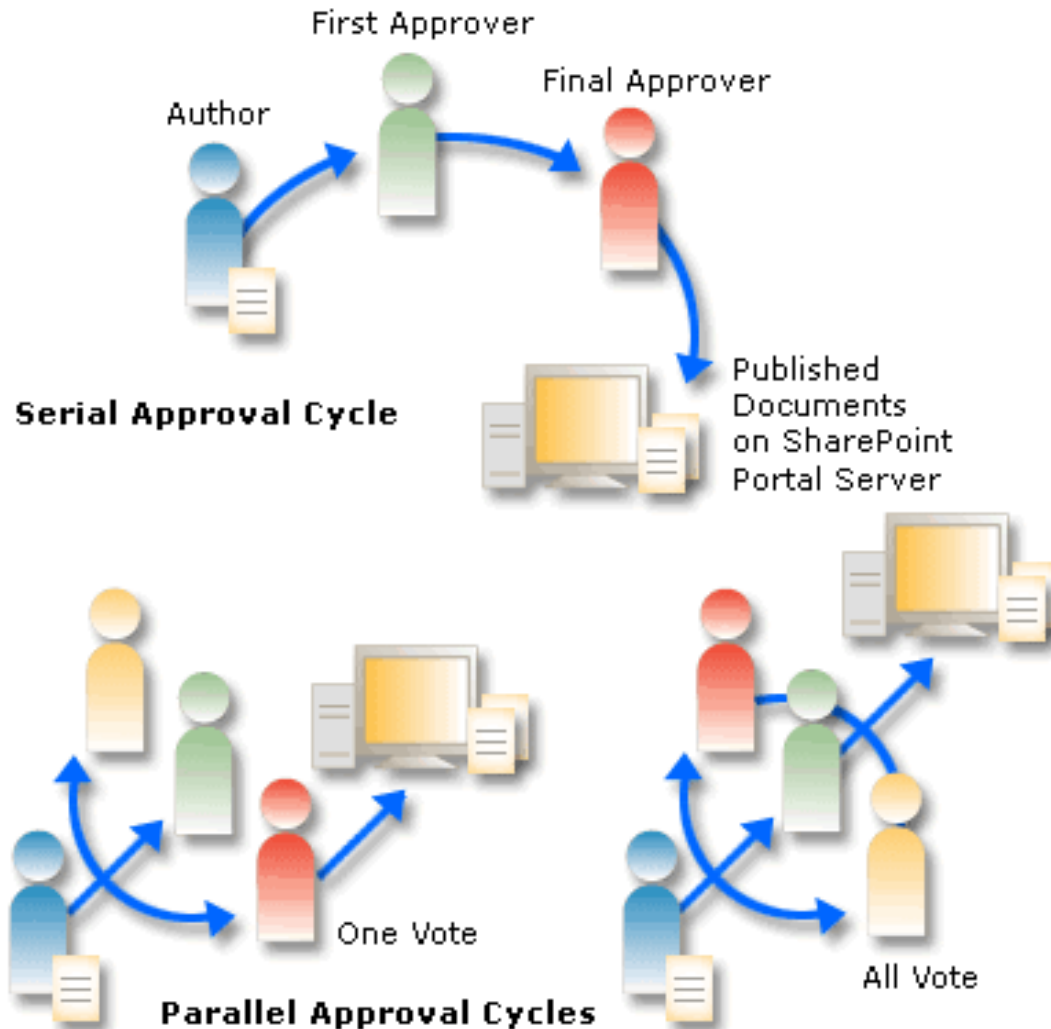
- Sites
- Document Workspaces
- Meeting Workspaces

This page shows all the lists in this Web site. Click the name of the list to view its contents. To create a new list, click Create List.

Create List

Lists	Description	Items	Last Modified
Announcements	Use the Announcements list to post messages on the home page of your site.	2	7 days ago
Contacts	Use the Contacts list for information about people that your team works with.	1	7 days ago
Events	Use the Events list to keep informed of upcoming meetings, deadlines, and other important events.	1	7 days ago
Links	Use the Links list for links to Web pages that your team members will find interesting or useful.	0	4 weeks ago
Tasks	Use the Tasks list to keep track of work that you or your team needs to complete.	1	6 minutes ago

Document Approval Cycle Types in Sharepoint



Approval Routing Setup in Sharepoint

As a coordinator on a folder, you can choose the approval route.

New Folder Properties [?] [X]

General | Security | Profiles | **Approval**

☒ Documents must be approved before publishing

Approvers:

Approver Name
1 - Jae Pak
2 - Lisa Jacobson

Add...

Route to approvers:

☒ One after another

☐ All at once



ADAPT Project Sharepoint New Alert Screen

New Alert - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media RSS Feeds Print Mail News Groups AutoFill Options

Address http://aet-srv/sites/adapt/_layouts/1033/SubNew.aspx?List={2F87B74D-F3A8-4898-870C-AA51B96D6EFE} Go Links

Google Search Web 446 blocked AutoFill Options

Home Documents and Lists Create Site Settings Help Up to ESA-AET

ADAPT

New Alert: Data Models: All items

Use this page to create an e-mail alert notifying you when there are changes to this item. [More information on alerts.](#)

<h3>Send Alerts To</h3> <p>All of your alerts will be sent to this e-mail address. Change my e-mail address.</p>	<p>My e-mail address is: tstaab@lanl.gov</p>
<h3>Change Type</h3> <p>Specify the type of changes that you want to be alerted to.</p>	<p>Alert me about:</p> <ul style="list-style-type: none"><input checked="" type="radio"/> All changes<input type="radio"/> Added items<input type="radio"/> Changed items<input type="radio"/> Deleted items<input type="radio"/> Web discussion updates
<h3>Alert Frequency</h3> <p>Specify whether you want to be alerted immediately when there is a change, or if you would rather receive a daily or weekly summary message.</p> <p>View my existing alerts on this site.</p>	<p>Alert me how often:</p> <ul style="list-style-type: none"><input checked="" type="radio"/> Send e-mail immediately.<input type="radio"/> Send a daily summary.<input type="radio"/> Send a weekly summary.

OK Cancel

ADAPT Project Sharepoint Tasks Screen

Tasks - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Reload Home Search Favorites Media RSS Print Mail News Groups

Address http://aet-srv/sites/adapt/Lists/Tasks/AllItems.aspx Go Links

Google Search Web 446 blocked AutoFill Options

Home Documents and Lists Create Site Settings Help Up to ESA-AET

ADAPT
Tasks

Select a View

- All Tasks
- My Tasks
- Due Today
- Active Tasks
- By Assigned To

Actions

- Add to My Links
- Alert me
- Export to spreadsheet
- Modify settings and columns

Use the Tasks list to keep track of work that you or your team needs to complete.

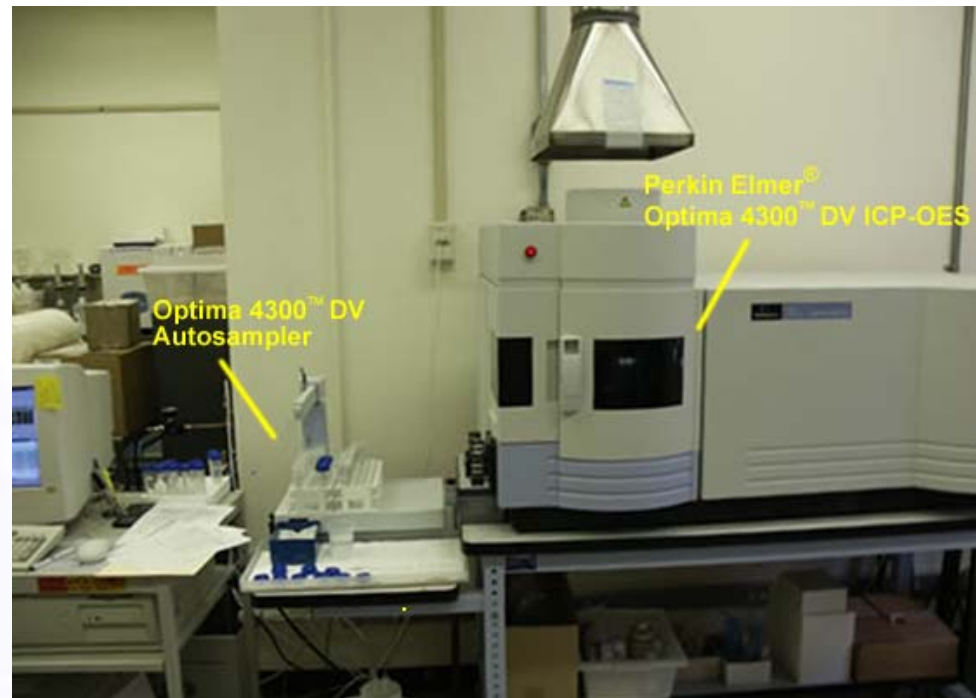
New Item Filter Edit in Datasheet

Title	Assigned To	Status	Priority	Due Date	% Complete
Develop Result Transfer Model NEW	Torsten A Staab	In Progress	(2) Normal		10%

Automating Instrument Data QC

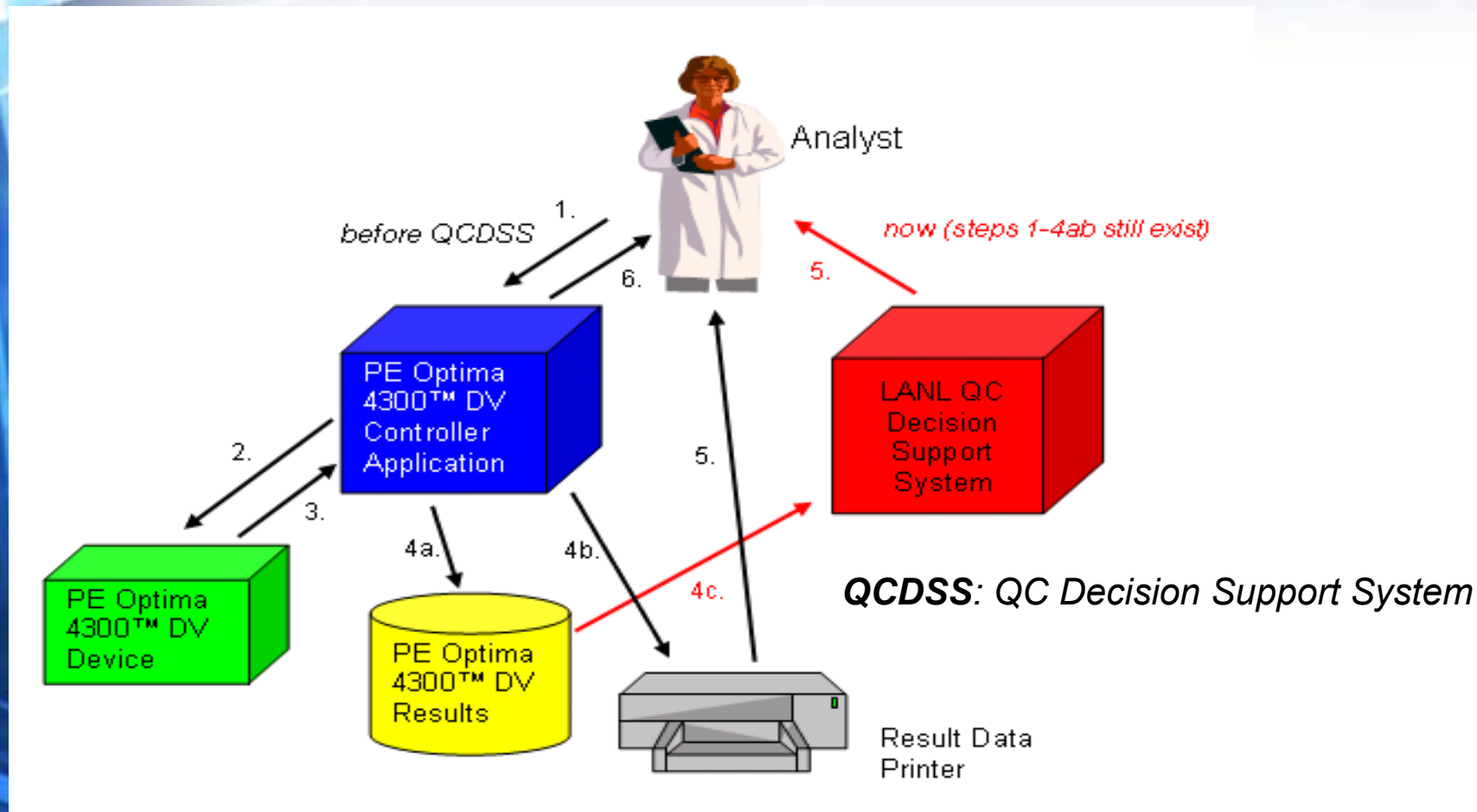
The Goal

Automate labor-intensive and time-consuming QC of instrument-generated analysis result data



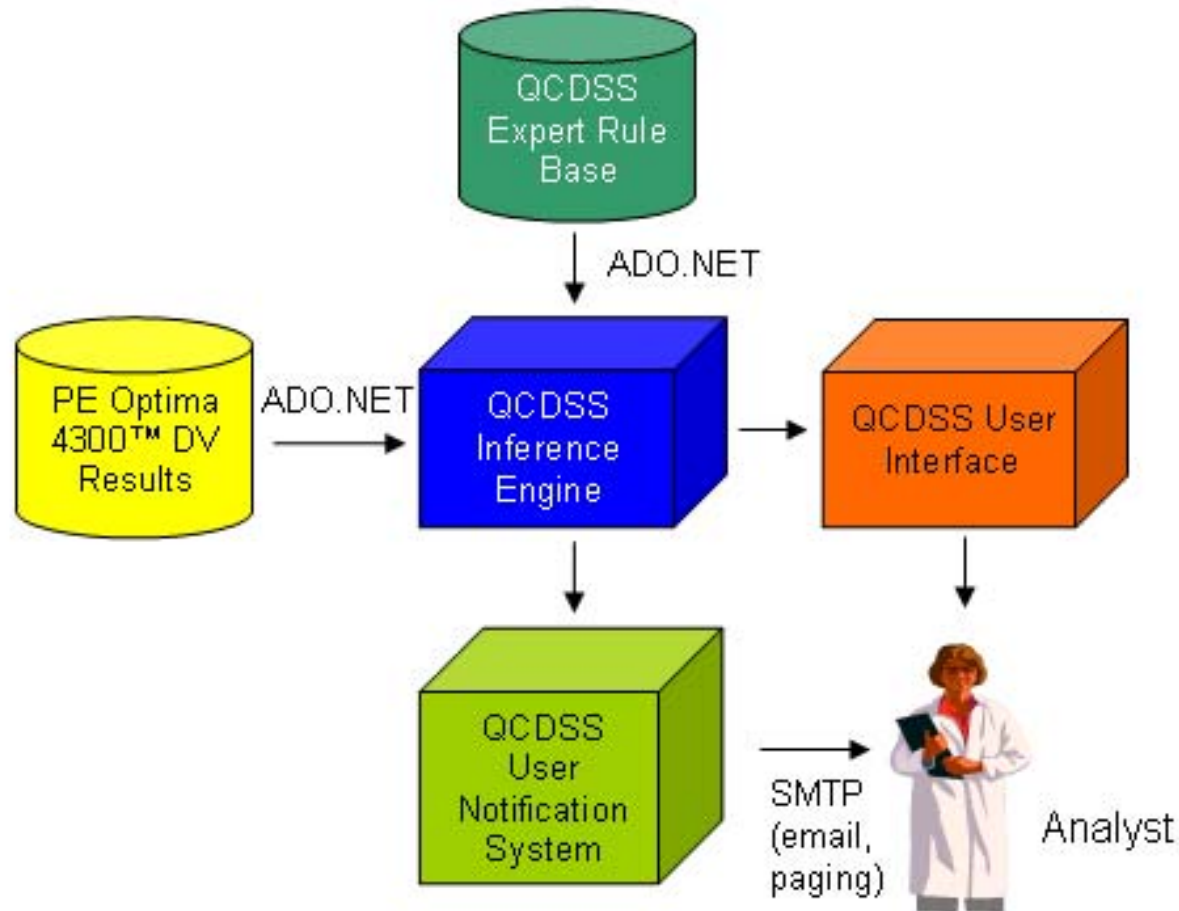
Automating Instrument Data QC

The System Architecture (1/2)



Automating Instrument Data QC

The System Architecture (2/2)



Automating Instrument Data QC

Screenshot of Software Prototype

LANL Optima QC V1.2

QC Dashboard | Config

Result Database: C:\Documents and Settings\Torst ... **Set**

Result Index: 659 8/7/2003 10:19:43 AM

☐ Generate Report

QC

	LCS		MS/MSD		RPD		PQL
	Low	High	Low	High	Low	High	
Al	0	0	76	113	-10	10	5.25
Be	83	105	80	109	-11	10	0.03
Cd	75	124	83	107	-5	5	0.30
Cr	85	110	81	111	-1	1	0.95
Cu	81	110	81	106	-6	6	0.95
Fe	82	118	79	123	-17	15	6.50
Ni	82	109	82	106	-7	6	0.65
Pb	75	106	81	105	-8	8	1.20
V	85	105	84	103	-3	2	0.40
Zn	69	142	74	128	-12	11	4.65
U385	0	0	80	120	-20	20	0.65
U409	0	0	80	120	-20	20	1.25

QC Tests

- ☐ BEC
- ☐ MNREPL
- ☒ CORRCOE
- ☒ ICV
- ☐ ICB
- ☒ PQLV
- ☒ ICS_A
- ☒ ICS_AB
- ☒ CCV
- ☒ CCB
- ☐ PREPBLAN

All **None**

Status

```
[1/20/2004 3:46:00 PM] done
[1/20/2004 3:46:00 PM] starting ICS_AB Check #8...
[1/20/2004 3:46:00 PM] [RED] (LogMean) ResultIndex: 659 SampleIndex: 9 MeanIndex: 106 QC va
[1/20/2004 3:46:00 PM] done
[1/20/2004 3:46:00 PM] starting CCV Check #9...
[1/20/2004 3:46:00 PM] done
[1/20/2004 3:46:00 PM] starting CCB Check #10...
[1/20/2004 3:46:00 PM] done
[1/20/2004 3:46:00 PM] starting PB100 Check #11...
[1/20/2004 3:46:01 PM] done
```

Analyses of Interest

- ☐ Al
- ☒ Be
- ☐ Cd
- ☒ Cr
- ☒ Cu
- ☒ Fe
- ☒ Ni
- ☒ Pb
- ☒ V
- ☒ Zn
- ☒ U385
- ☒ U409

All **None**

Exit **Clear**

Implemented in C#.NET and ADO.NET

QCDSS- generated, HTML-based QC Report

Prep Batch ID:	113	Analytes Requested:	Al, Cu, Fe	Results Data Set:	100
SDG#:	A34	Sample Type:	Metals	Analysis Date:	11/3/2003
Sample ID#s:	123, 456, 789	Analyst:	Torsten		

Acceptance Limits					Tests		
Analyte	LCS	MS_MSD	RPD	PQL	Description	Passed	Failed
Al	N/A	76-113	(-10) – (+10) %	5.25	1) Did BEC check pass (< 0.04)?	x	
Be	83-105	80-109	(-11) – (+10) %	0.03	2) Did Mn replicate test pass (< 2.0 % RSD)?	x	
Cd	75-124	83-107	(-5) – (+5) %	0.30	3) Is Correlation Coefficient >= 0.9950		x
Cr	85-110	81-111	(-1) – (+1) %	0.95	4) Did ICV pass (90-110%)?	x	
Cu	81-110	81-106	(-6) – (+6) %	0.95	5) Did ICB pass (-1 to 3x PQL)?		x
Fe	82-118	79-123	(-17) – (+15) %	6.50	6) Did PQLV pass (70-130%)?	x	
Ni	82-109	82-106	(-7) – (+6) %	0.65	7) Did ICS_A pass (-1 to 3x PQL)?	x	
Pb	75-106	81-105	(-8) – (+8) %	1.20	8) Did ICS_AB pass (80-120%)?		x
V	85-105	84-103	(-3) – (+2) %	0.40	9) Did CCV pass (90-110%)?	x	
Zn	69-142	74-128	(-12) – (+11) %	4.65	10) Did CCB pass (-1 to 3x PQL)?		x
U385	N/A	80-120	(-20) – (+20) %	0.65	11) Did Prep Blank pass (-1 to 3x PQL)?	x	
U409	N/A	80-120	(-20) – (+20) %	1.25	12) Did Media Blank pass (-1 to 3x PQL)?	x	
					13) Did LCS pass?		x
					14) Did MS recovery pass?	x	
					15) Did MSD recovery pass?		x
					16) Did MSD RPD pass?	x	
					17) Were standards and solutions current?	x	
					18) Did PB100 pass?		x
					19) Did Real Sample Measurement pass?	x	
					20) Did Rinse Blank pass?	x	

Standard Prep. Logbook ID#Page:

Prepared by:

Date prepared:

If "Failed" is checked, reference the number and describe the problem below:

- ☐ Be oversaturated
- ☐ Al without limits

Automating Instrument Data QC

Results of Automating Instrument QC

- LANL program performs QC in ~5 seconds as opposed to 20 minutes needed by human analyst
- improves sample analysis QC by eliminating potential for human error
- reduces laboratory operating cost; saves one Tech FTE per instrument per year
- minimizes device downtime and saves resources through a built-in, real-time, electronic notification system
- speeds up reporting by generating QC reports on-the-fly

Automating Instrument Data QC

Future Work

- apply same QC automation framework to other instruments
- store meta description of expert rules in a database and generate decision support system on-the-fly from stored rules
- LIMS Integration

Recent Paper: ***Improving Sample Analysis Throughout and Quality with a .NET-based, Real Time QC Decision Support System***, Torsten Staab, Toshiyuki Shiina, Derek Miller, Journal of the Association for Laboratory Automation (JALA), Elsevier Publishers, Vol 8/6, pp 107-112, December 2003.

Handheld Sample Collection & Tracking Device

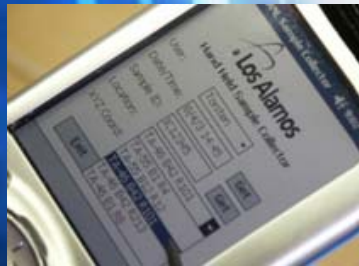
The Goals

- speed up indoor and outdoor sample collection (e.g., surface swipes with filter papers, contact plates, swabs, etc.) and minimize human error by automating the book keeping
- allow for cross contamination-free sampling
- minimize risk of human contact exposure
- reduce sampling costs

Handheld Sample Collection & Tracking Device

Technology Summary

Handheld device for multi-purpose indoor and outdoor sample collection & electronic sample registration.



Technology Components

- PDA / Wearable Computer
- Universal Sample Media Adapter
- Built-in Digital Camera
- 3D Location Tracking
- GPS
- Wireless Communication
- Voice Control
- Pressure Sensor etc.

1st Generation Prototype